CO 3.0 Technical and Scientific Viability - MRI will ensure the long-term viability of the Laboratory by building and enhancing NREL's technical capabilities.

NREL Proposed Grade: Outstanding

PO 3.1 Build, enhance, and sustain NREL's scientific, engineering, and analytic capabilities.

- PI 3.1.1 NREL technical capabilities are enhanced to effectively provide for long-term program needs and the Laboratory's sustainability and environmental goals (e.g., staff, facilities, and equipment that enable science and technology work at NREL):
 - Staff expertise strategic hires, DDRD projects, key staff additions and staff development assignments, training, and experiences
 - Facility capabilities enhancements to existing facilities and/or completed milestones in constructing/operating new facilities that represent added capability
 - Equipment enhancement and/or addition of scientific equipment; new concepts/areas of expertise DDRD investments and outcomes.

Assessment Summary

NREL continues to enhance its technical capabilities in support of strategic program and national needs through focused investments in staff, equipment, facilities and ideas. Through internal investments in exploratory research, NREL continues to substantially extend the scientific and technical capabilities necessary to support long-term program needs, national energy goals, and national environmental sustainability goals. As a result of program support and strategically selected investments, NREL strengthened its long-term capabilities in computational sciences by acquiring a chemistry package that will help advance several different research areas at the Lab. Analytical equipment was expanded or purchased to provide new tools that enable state-of-the-art measurements and resulting data.

NREL's vision for the future of its physical sites was demonstrated by the completion of the 25-year NREL General Development Vision, which provides the framework for developing the South Table Mountain Site and National Wind Technology Center. This plan will be instrumental in guiding the



Among the instruments purchased for the new Biomass Surface Characterization Laboratory was a scanning electron microscope, which will be used for composition analysis, topographic imaging, and structural microcharacterization.

Lab's strategic investments in future buildings and infrastructure. NREL's next major research building, the S&TF (discussed under Critical Outcome 4.0) will provide a unique capability to develop advanced technologies for thin-film and nanostructure fabrication in support of renewable energy and energy efficiency goals. NREL also developed plans for key additions of critically needed new facilities at the National Wind Technology Center.

Biomass Capabilities

Development of Biomass Surface Characterization Laboratory Initiated. The NREL and DOE Biomass Program have committed to establishing a very unique facility at NREL for the advanced characterization of biomass surfaces (materials). NREL used \$2.2M in capital funds provided by OBP to purchase microscopy equipment to build a world-class Biomass Surface Characterization Laboratory. These new surface tools greatly characterization enhance NREL's resources for developing improved biomass

pretreatment technology and improved enzymes for cellulose and hemicellulose hydrolysis. Among equipment purchased for the new laboratory were:

- Scanning electron microscope for compositional analysis of samples, topographical imaging, and structural microcharacterization.
- Transmission electron microscope for high-resolution imaging, and structural, compositional, and cross-sectional analysis.
- Near-field optical microscope for fundamental material and nanoscale studies.

The Biomass Surface Characterization Laboratory will keep NREL at the cutting edge of botany, biochemistry, chemistry, and material and computer sciences. It will also help DOE achieve the long-term goal of developing biorefineries to produce fuels, chemicals, and biobased products from lignocellulosic biomass that are cost competitive with petroleum-derived.

Computational Sciences Capabilities

Computation Chemistry Package Available for use at NREL. NWChem has been installed and made available to NREL scientists on the NREL IBM highperformance computing system. NWChem is a computational chemistry package. It is designed to run on parallel supercomputers and to treat large problems efficiently. In addition, the companion software Extensible Computational Environment (Ecce) has also been installed. It provides a sophisticated graphical user interface, scientific tools. underlying visualization and the management framework enabling scientists efficiently set up calculations and store, retrieve, and analyze the rapidly growing volumes of data produced by computational chemistry studies. These software packages add to the capabilities of NREL.

Visualization Capabilities Enhanced Based on Workshop Results. NREL held its first workshop on Computational Science in Biology, Chemistry & Materials Science on April 3rd. The workshop focused on common needs and challenges in numerical modeling and simulation for scientists - the most pressing of which was a requirement for scientists to be able to visualize the results of their scientific simulations. In response to this expressed need, NREL specified and purchased a stereoscopi, 3-D visualization system. This system, which is currently being installed and tested, will greatly enhance NREL's scientific modeling and will aid scientists in accelerating their research and in understanding basic phenomenal processes.

Strategic Hire Augments Computer Programming Capabilities. The hire of Mr. Peter Ellis was made to augment our capability in computational sciences for building energy simulations. Ellis comes to NREL with experience as a mechanical engineer and in computations. The retirement of a research fellow working in this area and a transition to an emphasis on EnergyPlus were the drivers for this hire and will keep NREL in a leadership role in building energy simulation and in communicating the scientific results.

Distributed Energy and Electric Reliability Capabilities

Test Facility gets new Inverter Test Bed. NREL completed construction of an inverter test bed at the Distributed Energy Resource Test Facility (DERTF). This test bed contains 13 inverters and will be used to test the response of multiple distributed resources to abnormal utility conditions. This work will provide valuable insight into the impacts of large numbers of distributed resources on single distribution feeders and will add to the capability to test multiple inverters at the DERTF.



New test bed at the Distributed Energy Resource Test Facility contains thirteen inverters and will be used to test the response of distributed resources to abnormal utility conditions.

Advanced Thermal Conversion Lab Receives *Upgrades*. NREL commissioned the second test station at the Advanced Thermal Conversion Lab for highspeed testing of full-scale waste heat recovery, HVAC (heating, ventilation, and air-conditioning), and aircleaning technologies, and has already used the test station to complete the evaluation of 16 new heat recovery and dehumidification devices. Among the upgrades made to the lab is the addition of automated contaminant samplers originally developed under NREL's DDRD Program (Director's Discretionary Research and Development), which are being applied to the development of next-generation air cleaners. Additional upgrades to the lab provide the ability to precisely, quickly, and accurately evaluate new fullscale VOC (volatile organic compound) filters. These upgrades enable researchers to develop improved thermally activated technology (TAT) components, facilitate the integration of components into energy efficient systems to ensure effective environmental quality, and provide DOE with in-depth understanding of the state-of-the-art of TAT HVAC and waste-heat recovery technologies.

FreedomCAR and Vehicle Transportation Capabilities

Toxic Measurements Capability Added. NREL added the capability to measure toxic emissions at its ReFUEL laboratory, which will increase researchers' understanding of the impacts and compliance of advanced engines and fuels for high fuel-efficiency transportation. A gas chromatograph (GC) will enable researchers to speciate and quantify emissions of C1-C12 hydrocarbons — including 1,3-butadiene and

benzene. Both of these chemicals are carcinogens and are being considered by the California Air Resource Board for future regulation. A high-performance liquid chromatograph (HPLC) will quantify emissions of aldehydes and ketones, which are pulmonary irritants.



A new liquid chromatograph in NREL's ReFUEL laboratory allows researchers to analyze aldehyde emissions.

Energy Storage Lab

Gains New Capabilities. The energy storage team added new experimental capabilities to its laboratory. The team:

- Acquired a unique, custom-made AC power amplifier for testing battery pre-heating concepts for vehicles that operate in cold climates and evaluating the effects of high-frequency harmonics on battery life.
- Designed and installed anode testing equipment for quickly screening the effectiveness of anodes with different materials and designs.
- Designed and fabricated a device to measure the thermal conductivity of battery materials, an important parameter for battery thermal analysis.
- Designed a new battery calorimeter for measuring heat generation from batteries, information essential for proper thermal management of batteries.

Laboratory Flexibility and Capability Upgrades for Future Generations of Engines and Vehicles. The ReFUEL laboratory control and data acquisition systems were upgraded to modern, more flexible PC-based technology. These upgrades significantly improve the ability of the lab to be reconfigured to meet new test protocols in the demanding and rapidly evolving field of heavy-duty vehicle research. The lab was also refurbished to enable it to meet the 2007 emission measurement testing standards. The most

significant of the changes was the installation of the Class 1000 clean room for particulate matter metrology, which features precise environmental controls for conditioning particulate matter filters prior to measurement.



New Class 1000 clean room for particulate matter metrology for ReFUEL lab.

Distributed Computing Capability Built $ADVISOR^{\mathsf{TM}}$. With the installation of the distributed computer program "Condor" on twenty personal computers, NREL's vehicle systems analysis team enhanced its analytical tools. This initial cluster includes both dedicated and staff-used workstations, including processors ranging from 500 MHz to 2.8 GHz. The system greatly increases the utilization of computational power by storing jobs that need to be run in a queue and then executing them on available machines. Plus, the DIRECT optimization routine that was used extensively with ADVISOR™ was modified to exploit the distributed computing resources. As an indication of the power of this new analytical computing capability, it was tested on a fuel-cell vehicle design problem using ADVISOR[™]. In this analytical test, more than 1,000 hours of computational time were completed in 72 hours of clock time.

Hydrogen, Fuel Cells, and Infrastructure Technologies Capabilities

New XRD Facility. NREL established a new X-ray diffraction (XRD) facility that will improve capabilities. The new facility will allow mapping of large samples, screening of combinatorial samples, and in situ thermal processing of samples.

New Capabilities for Synthesizing Carbon Nanotubes. NREL has developed two new capabilities for synthesizing single-wall carbon nanotubes (SWNTs). The first is the addition of a heated arc-discharge synthesis reactor. The second, a capability derived from a DDRD project, is the development of a hot-wire chemical vapor deposition system for SWNTs. Besides

being very promising for hydrogen storage, SWNTs also have potential applications for gas separations, fuel-cell membranes, batteries, photovoltaics, composite materials, nanoscale wires, and more. The promise of these approaches for making SWNTs is that they are continuous production techniques, which has great advantages over NREL's currently available laser-based batch processes.

NREL General Development Vision (Site Planning and Development)

NREL Delivers Completed Site Development Vision to DOE and Management. NREL completed the 25-year General Development Vision for both the South Table Mountain campus and the NWTC campus. The development of the plan involved discussions with more than 150 of NREL's managers, and staff members. The planning process also included site planning consultants, members of NREL's Advisory Board, architects and engineers, meetings, workshops, and reviews. This plan will provide the framework for developing NREL's sites over the next 25 years. The plan was documented in draft reports that were orally presented to:

- The NREL design advisory board in May
- NREL executive management in June
- MRI board of governors in July

A revised draft report that incorporated comments from previous reviews was presented to GO and NREL executive management in August 2003. A final report incorporating the latest review comments is now being prepared and will be ready by the end of October 2003.



Artist rendition of completed South Table Mesa campus as seen from the east entrance.

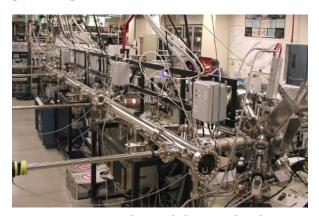
Quality Assurance

Attaining ISO Accreditation. NREL made significant contributions to building the Laboratory's technical capabilities and long-term viability by obtaining/retaining ISO 17025 accreditation. ISO

17025 accreditation is important to NREL because it is the internationally recognized standard for testing and calibration laboratories. Having this accreditation acknowledges that the Laboratory has a quality system in place that enables it to deliver testing and calibration results of known quality. NREL developed needed documentation and training, and performed quality audits that enable the NWTC Certification Team to maintain its ISO 17025 accreditation, and to gain accreditation for the NCPV Solar Cell/Module Group's testing and calibration.

Solar and Solid-State Materials Research

Tool Surface Analysis **Process** Integration Developed and Installed. For the surface analysis lab in the Solar Energy Research Facility (SERF), NREL designed and installed a system that integrates Auger and XPS analysis systems with a surface modification and deposition workstation, and a glove box. This new tool enables a semiconductor surface of a device to be deposited, analyzed for elemental and chemical composition, and then modified all in one, interconnected, clustered system. The heart of the design is a vacuum transport system that conveys the semiconductor device from station to station without exposure to ambient atmosphere. The development of this tool serves as a prototype for more elaborate capabilities planned for the new S&TF.



New NREL custom designed cluster tool in the surface analysis lab combines Auger and XPS characterization capability with deposition

Single-crystal X-ray Diffraction Facility. Under a DDRD project, NREL established the capability to perform X-ray diffraction measurements and analyses on single crystals. This provides NREL with a fundamental analytical capability to ascertain the crystalline structure of new materials, which is especially important for photovoltaic and solid-state technologies.

New Diagnostic Capability for Characterizing Nanostructure Matter. Under a DDRD project, NREL is establishing a new capability to characterize the energy levels of individual nanoparticles and the dynamics of interparticle charge transport among assemblies of these nanoparticles. This new capability arises from a unique approach of combining interrelated diagnostic techniques — low-temperature and ambient tunneling spectroscopy, photocurrent transient spectroscopy, and electrochemical transistor setup. This new capability will yield insight into the interplay between the energy structure of single particles and the charge transport among particles. As part of this project, a new low-temperature AFM/STM instrument was purchased and installed.

Wind Energy Capabilities

Planning for Large Wind Turbine Test Facility. NREL Site Operations and the NWTC have continued to move plans forward for building the Large Wind Turbine Test Facility. This is a facility that would house an 8-MW dynamometer and a 70-meter bladetesting area to accommodate the testing of the latest generation of MW-scale wind turbine components being developed by the wind industry. The efforts thus far this year have included the development of Critical Design 0 and OMB 300 submittal packages, budget and schedule estimates for DOE management review, and briefings to explain the requirements and need for such a facility. NREL has involved key industry members in a dialog to ensure the facility meets the requirements of the industry.